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      7
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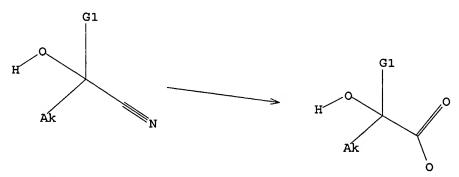
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PROJECTED VERIFICATIONS:

7598 TO

10122

PROJECTED ANSWERS:

5 TO

132 HIT RXNS (

1.2

L3

5 SEA SSS SAM L1 ( 5 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 14:53:23 FILE 'CASREACT'

SCREENING COMPLETE - 12399 REACTIONS TO VERIFY FROM 1213 DOCUMENTS

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=> s 13

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=> s 13 not py > 2004

87 L3

3993509 PY > 2004

L566 L3 NOT PY > 2004

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L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:242505 CAPLUS

DOCUMENT NUMBER: 140:423490

TITLE: Synthesis of the marine compound (2R,5Z,9Z)-2-

methoxyhexacosa-5,9-dienoic acid via a

lipase-catalyzed resolution and a novel O-alkylation

protocol

AUTHOR(S): Kulkarni, Bheemashankar A.; Sharma, Anubha; Gamre,

Sunita; Chattopadhyay, Subrata

CORPORATE SOURCE: Bio-Organic Division, Bhabha Atomic Research Centre,

Mumbai, 400 085, India

SOURCE: Synthesis (2004), (4), 595-599

CODEN: SYNTBF; ISSN: 0039-7881 Georg Thieme Verlag

PUBLISHER: Georg
DOCUMENT TYPE: Journa

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:423490

AB The title compound has been synthesized by a facile route starting from 4-pentyn-1-ol. The enantioselectivity was attained by a strategy involving a lipase-catalyzed acetylation of a solid-phase immobilized long chain  $\alpha$ -hydroxy acid. Another important feature of the synthesis was the formulation of an efficient HgO-catalyzed O-methylation of the  $\alpha$ -hydroxy acids which proceeded without any racemization. The alkylation protocol was also highly efficient for selective

mono-methylation/benzylation of sym. diols.

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:688298 CAPLUS

DOCUMENT NUMBER: 140:320064

TITLE: Biocatalytic hydrolysis of cyanohydrins: an efficient

approach to enantiopure  $\alpha$ -hydroxy carboxylic

acids

AUTHOR(S): Osprian, Ingrid; Fechter, Martin H.; Griengl, Herfried

CORPORATE SOURCE: Institute of Organic Chemistry, Graz University of

Technology, Graz, A-8010, Austria

SOURCE: Journal of Molecular Catalysis B: Enzymatic (2003),

24-25, 89-98

CODEN: JMCEF8; ISSN: 1381-1177

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:320064

AB Rhodococcus erythropolis NCIMB 11540 was found to have a highly active nitrile hydratase/amidase enzyme system present which accepts the nitrile function of α-hydroxynitriles (cyanohydrins) as substrates. This biocatalytic hydrolysis using whole bacterial cells leads to α-hydroxy carboxylic acids which are much valued chiral building blocks in organic synthesis. Employing enantiopure cyanohydrins, which are easy available using (R) - or (S)-hydroxynitrile lyases, the products were obtained in high yield without racemization, decomposition or side reactions. Herein, the application of this biotransformation for preparative scale applications is described. To clarify the substrate acceptance of the nitrile hydrolyzing enzymes of R. erythropolis NCIMB 11540, several selected model compds. were subjected to biocatalytic hydrolysis.

Reaction conditions were optimized to enable preparative scale conversions. In this manner, (R)-2-chloromandelic acid and (R)-2-hydroxy-4-phenylbutyric acid, two important pharmaceutical intermediates, were prepared in a gram scale. The substrate concns. used were 9.3 and 13 g/l, resp. The process yielded both acids in high optical (ee>99 and 98%) and chemical (98%) yield after short reaction times (3 and 1.5 h).

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:90001 CAPLUS

DOCUMENT NUMBER: 136:134502

TITLE: Process for producing 2-hydroxy-4-methylthiobutanoic

acid

INVENTOR(S): Ikudome, Kenji; Shiozaki, Tetsuya; Otani, Takehiro;

Sudo, Shogo

PATENT ASSIGNEE(S): Sumitomo Chemical Company, Limited, Japan

SOURCE: PCT Int. Appl., 15 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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APPLICATION NO.
    PATENT NO.
                  KIND DATE
    WO 2002008181 A1
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                             20020131 WO 2001-JP5982
                       A1
                                                             20010709
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
           CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
           HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
           MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE,
            SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA,
            ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
           DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
           BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                             20020206 JP 2000-223436
    JP 2002037769
                       A
                                                              20000725
PRIORITY APPLN. INFO.:
                                        JP 2000-223436
                                                          A 20000725
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CASREACT 136:134502 OTHER SOURCE(S):

This document discloses a process for producing 2-hydroxy-4methylthiobutanoic acid which comprises hydrating 2-hydroxy-4methylthiobutanenitrile in the presence of sulfuric acid, hydrolyzing the 2-hydroxy-4-methylthiobutanamide contained in the reaction mixture, subsequently separating the resultant reaction mixture into an oil layer containing

2-hydroxy-4-methylthiobutanoic acid and an aqueous layer, and circulating a part of the aqueous layer to the hydrolysis step and/or the oil/water separation

step. By the process, 2-hydroxy-4-methylthiobutanoic acid can be efficiently obtained in a satisfactory manner without using an organic solvent.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1992:591348 CAPLUS

DOCUMENT NUMBER: 117:191348

TITLE: Preparation of  $\alpha$ -hydroxyisobutyric acid by

hydrolysis of acetone cyanohydrin

INVENTOR (S): Noguchi, Shizuo; Ogiwara, Shinei; Nakamura, Akira

PATENT ASSIGNEE(S): Kuraray Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

KIND PATENT NO. DATE APPLICATION NO. DATE --------------------JP 04193845 A 19920713 JP 1990-324957 19901126 JP 2909198 B2 19990623

PRIORITY APPLN. INFO.:

JP 1990-324957 19901126

OTHER SOURCE(S):

CASREACT 117:191348 In preparation of Me2C(OH)CO2H (I) by hydrolysis of Me2C(OH)CN (II) with HCl,

1:(1.0-1.5):(3.6-5.4) mol. ratio of II, HCl, and H2O are heated at 65-95° and optionally II is extracted by organic solvents. II (17.0 g) was added to 23.0 g 36% aqueous HCl, stirred at 80-90° for 2 h, and extracted with iso-Pr ether to give 97% I.

L6 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1950:20099 CAPLUS

DOCUMENT NUMBER: 44:20099

ORIGINAL REFERENCE NO.: 44:3993h-i,3994a-i

TITLE: Addition and condensation reactions of 2-pyridone

AUTHOR (S): Adams, Roger; Jones, Viron V.

SOURCE: Journal of the American Chemical Society (1949), 71,

3826-33

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: LANGUAGE:

Journal Unavailable

OTHER SOURCE(S):

CASREACT 44:20099

For diagram(s), see printed CA Issue.

CH2:C(NHAc)CO2H (0.5 g.) and 0.5 g. 2(1H)-pyridone (I), heated 1 hr. at 140°, give the Ac derivative (II), m. 199° (m.ps. corrected), of  $\alpha\text{-amino-2(1H)-pyridone-1-propionic acid, m. 236° (decomposition)}$  (72% from II on refluxing 6 hrs. with 48% HBr). 2(1H)-Pyridone-1propionic acid (III) (15 g.), 3.6 g. red P, and 30 ml. CCl4, treated dropwise at 0° with 60 g. Br and gradually heated to remove HBr, give 32% 3,5-dibromo-2(1H)-pyridone-1-propionic acid, m. 182°. Cl-CH2CH(OMe)2 (20 g.) and 10 g. H2O containing 10 drops concentrated HCl,

refluxed

until the 2 phases disappear, treated with 10 g. I, refluxed an addnl. hr., the volatile products distilled at 100°/20 mm., and 50 ml. Me2CO added, give 66% 2(1H)-pyridone-1-acetaldehyde-HCl, m. 139-40°; the free base (IV) is a sirup which yields an oxime, m. 78-9°, and a semicarbazone, m. 155-6°; IV could not be converted to an amino acid. BrCH2COCO2H and I, kept 10 hrs. at 55° and the residue in Me2CO treated with a small quantity of HBr, give a compound m. 143-5° (decomposition), which may be the 2-pyridonium salt of 2(1H)-pyridone-1-pyruvic acid-HBr; it yields II picrate in EtOH. I (5 g.) and 7 g. butadiene sulfone in 50 ml. absolute EtOH containing KOH, refluxed 2 hrs., give 73% of

the

adduct C9H11NO2S, m. 136-7°; I does not add mesityl oxide. The Na salt of I (with 2 mols. H2O) (20 g.) and 30 g. BrCH2CHBrCO2H in 50 ml. Me2CO, heated on the steam bath, the solvent evaporated, the residue extracted with MeNO2, and the extract diluted with ether, give 64% of a H2O-soluble

compound (V), with 1 mol. H2O, m. 122-3°. V (6 g.) results also from 12 g. of the Na salt of I and 28 g. BrCH2CHBrCO2Et in EtOH (refluxing 15 min.), followed by hydrolysis, and in 70% yield from I and CH2:CBrCO2H (heating 1 hr. on a steam cone) and in 4.5-g. yield from 9.5 g. I and 18 g. CH2:CBrCO2Et. V (2 g.) and 20 ml. concentrated NH4OH, refluxed 1 hr., give 71%  $\alpha$ -2(1H)-pyridone- $\beta$ -aminopropionic acid (VI), m. 213-15° (decomposition); 0.35 g. VI in 2 ml. absolute EtOH, treated with HBr until solution results, gives 89% of the lactam-HBr of VI, m. 298-9° (decomposition); with NH4OH it yields VI. VI (0.8 g.) and 0.5 g. NaOH in 5 ml.

H2O, refluxed 0.5 hr., give 52%  $\alpha$ -[2(1H)-pyridone]- $\beta$ hydroxypropionic acid (VII), m. 173-5°; this results in 79% yield from V and NaOH in H2O (refluxed 1 hr.); VII is unchanged on refluxing with 48% HBr 4 hrs. The Ac derivative of VII m. 224-5° (39%). O.CH2.CHCO2H (1.3 g.) and 0.95 g. I in 2 ml. EtOH, heated 1 hr. on the steam cone, give 55% VII. V (2.6 g.) in 20 ml. MeOH, macerated 2 min. with Ag20 (1.7 g. AgNO3), gives 56% of the hydrate, m. 105-7°, of the betaine (VIII), C8H7NO3, m. 159-65°; HBr regenerates V. V (2 g.) in 100 ml. hot 95% EtOH, hydrogenated over Pd-C at 50°/50 lb. and the resulting sirup in 50 ml. MeOH saturated with NH3, give 0.5 g.  $\alpha$ -(2-piperidone)- $\beta$ -aminopropionic acid, with 1 mol. H2O, m. 177-9°; further reduction over Pt oxide gives VI. V (4 g.) and 50 mg. Pt oxide in 100 ml. EtOH, hydrogenated at 50°/50 lb., give 83% of the HBr salt, m. 173-4°, of  $\alpha$ -hydroxy-1piperidinepropionic acid (IX), m. 219-20°; 48% HBr (refluxed 4 hrs.) gives the HBr salt; 5 g. IX and 1 ml. 48% HBr in 50 ml. MeOH, refluxed 12 hrs., give 86% of the Me ester-HBr, m. 141°; the free ester could not be obtained, Ag20 in MeOH giving IX. Pyrolysis of IX.HBr at 175-85°/1 mm. gives 88% piperidine-HBr. Piperidine and ClCH2CH(OH)CO2H, heated 1 hr. on the steam bath, give 55% IX. 1-Piperidineacetaldehyde-HCl (15 g.) in 15 ml. H2O, added to 1.5 g. NaCN in 25 ml. H2O, gives 95% lpha-hydroxy-1-piperidinepropionitrile, m. 97-8°; hydrolysis with concentrated HCl (refluxing 4 hrs.) gives 92% IX. III (2 g.) in 100 ml. 95% EtOH, hydrogenated (18 hrs.) over Pd-C at room temperature/40 lb., gives 70% 2-piperidone-1-propionic acid, m. 148° [HBr salt, m. 179° (decomposition)]. The Na salt of I (5.8 g.) and 8.8 g. MeCHBrCO2Me in 25 ml. absolute EtOH, refluxed 1 hr. and the sirup saponified by heating 1 hr. with 4 g. NaOH in 10 ml. H2O, give 93%  $\alpha$ -2(1H)pyridonepropionic acid (X), m. 215-17° (decomposition); catalytic reduction over Pt oxide gives 93%  $\alpha$ -2-piperidone-1-propionic acid, m. 144°. The Na salt of I (5 g.) and 8 g. EtOCH2CHBrCO2Et in 25 ml. absolute EtOH, refluxed 4 hrs., give 12%  $\alpha, \beta$ -bis(2(1H)pyridone)propionic acid, m. 151°. Infrared spectra are given for V, VIII and its HBr salt, 2(1H)-pyridonepropionic acid, 2-propoxypyridine, and 1-propyl-2(1H)-pyridone.